

# **ORIGEN-S AND ORIGEN-ARP: TIPS AND TRICKS**

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# INTRODUCTION

There are few codes I have seen that are more cryptic and more difficult to deal with than ORIGIN-S. Incidentally, most of the worse ones also come distributed with the SCALE package by the RSICC. The data input is an arcane relic from the days of Fortran, with an 80-character line limit and very little non-numerical text to be seen. Every control parameter for the program is input as a sequence of numbers, which the ORIGIN-S manual calls a “vector”. This format does nothing to explain what each of the elements in a vector represent, necessitating a long slog through a very ungainly technical manual. Figuring out the hundreds of numerical inputs that an ORIGIN-S file requires takes days.

Luckily, there is a big shortcut in the form of ORIGIN-ARP. This program was written to ease the use of ORIGIN-S by translating data entered in a graphical interface into the vectors that make up an ORIGIN input deck. While much better than the alternative, ORIGIN-ARP is not perfect, and imposes some rather irksome limitations on the user. This guide aims to help a user overcome such technical hurdles.

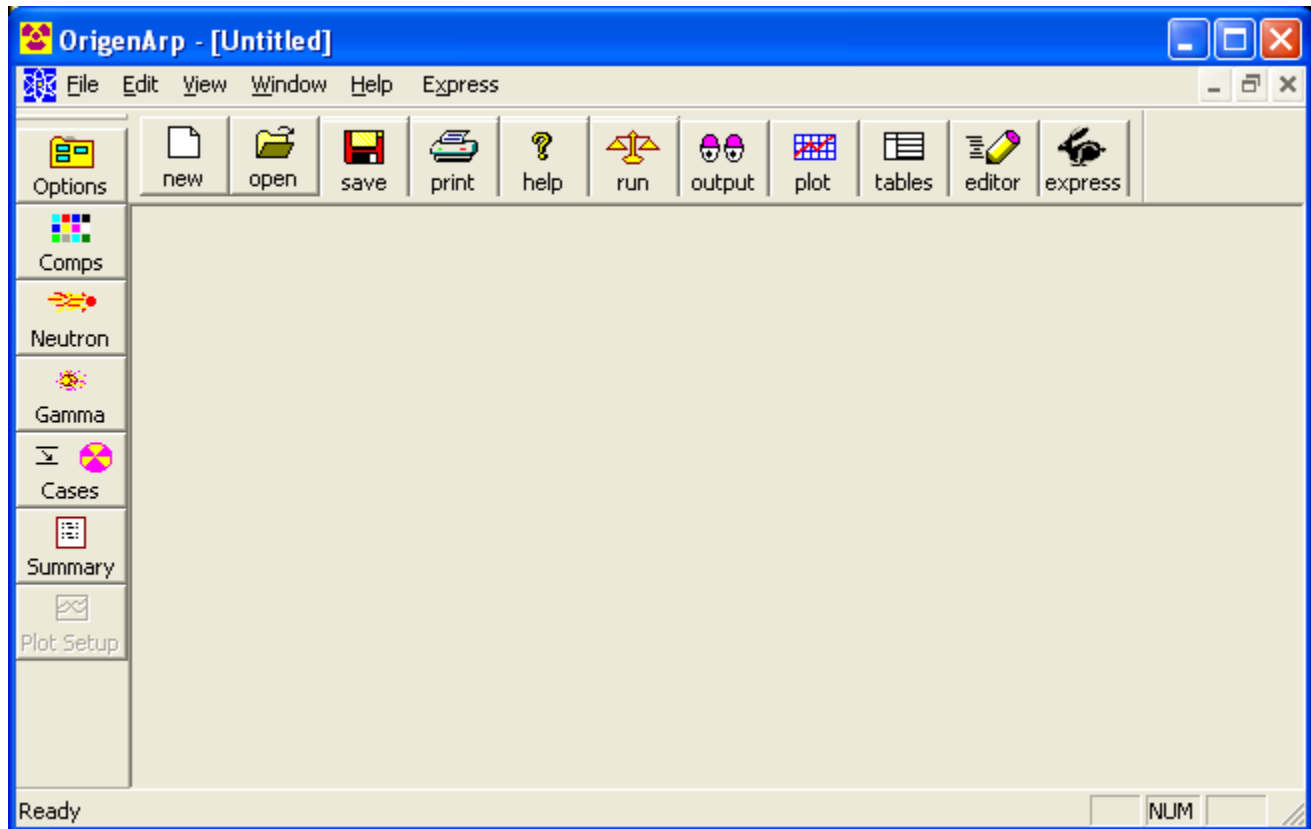
Note that the ARP interface can execute input files that it has loaded for editing. There are two other ways to execute an ORIGIN-S task. First, dragging an ORIGIN-S input file onto a shortcut to the “Run SCALE6” shortcut calls ORIGIN in batch mode. Alternately, from a command line, one can submit

**C:\\WINDOWS\\system32\\cmd.exe /k C:\\scale6\\cmds\\runscale.bat [INPUT\_FILENAME]**

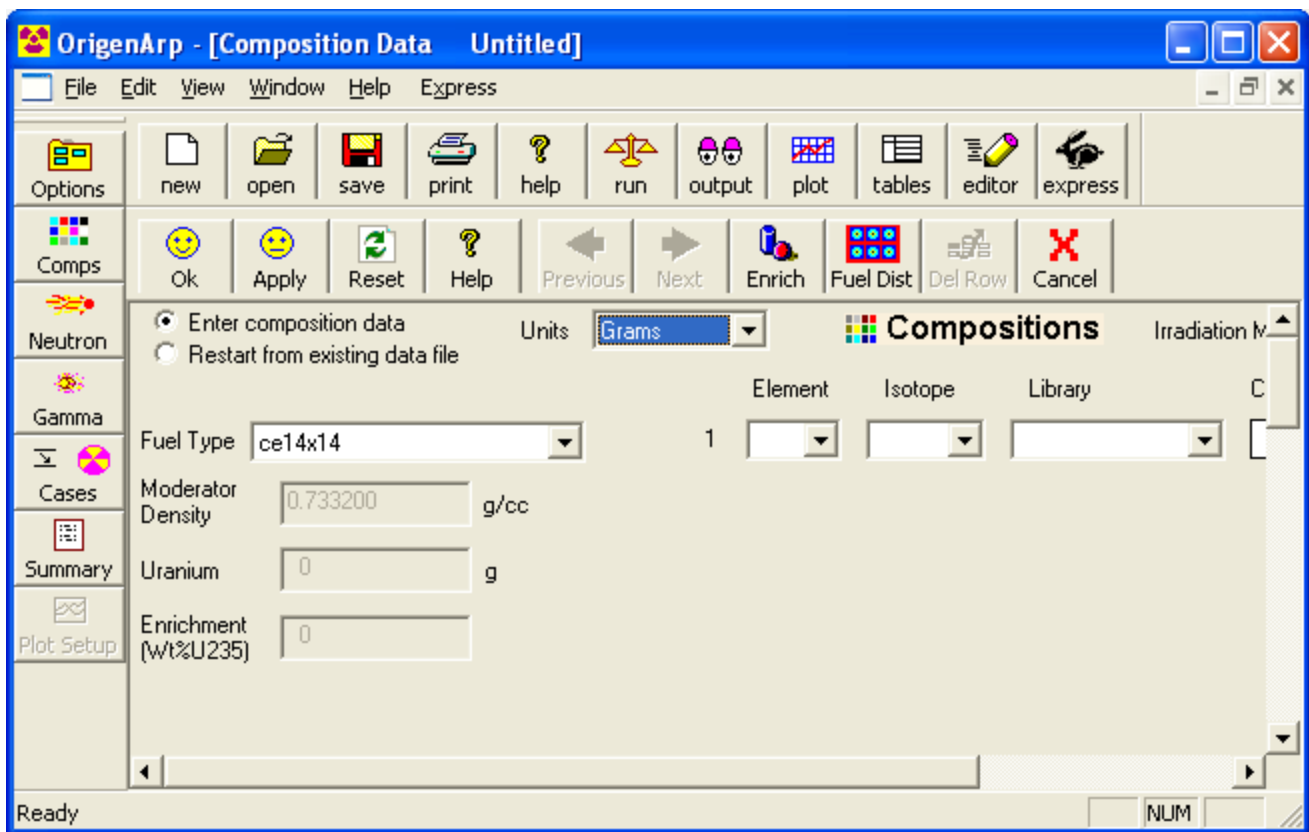
to do the same thing. This does assume that SCALE is installed to C:\\SCALE6.

## THE INTERFACE

I will begin with an introduction to the ORIGEN-ARP interface. It is not what one would call a professional job--animated smiley faces and other nonsensical icons have no place in a nuclear engineering tool. Still, it does the job and is fairly easy to navigate.



The main data entry is grouped into a set of 7 tabs on the left-hand side of the window. Pressing on one of the tabs opens a sub-window like the one below:



**After entering data for any of these sections, note that you must click the “OK” smiley button to save your work!** Make sure all the tabs are closed before saving to file, as the data from open tabs may not be recorded.

One of the great things about ORIGEN-ARP is that you don't need to define every field on every tab. The interface takes care of \*most\* of the default settings that a given simulation requires to execute. If there is missing input that ORIGEN cannot use a default for, it will prompt you to enter data manually for that field. Entering data can be a bit trying, since the program does not seem to support the Windows standard Ctrl+C and Ctrl+V copy/paste hotkeys. Be prepared to do a lot of left-clicking on drop-down menus.

# DATA ENTRY IN ORIGEN-ARP

Without further ado, here is a brief explanation of the various options and variables at your disposal in ORIGEN-ARP. I have organized this section into 7 groups, each corresponding to one of the main data-entry tabs.

## 1. OPTIONS

Generally speaking, you should not need to change anything on this tab. The most important option toggles between the “Fuel Irradiation” and “Activation” modes, but you are asked to specify this when starting ORIGEN-ARP.

- **“Maximum number of energy groups”**

Defines the number of energy bins used for radiation spectra. This is automatically set when you define your group structure in the “Gamma” and “Neutron” tabs.

- **“Number of columns for energy groups”**

Specifies the number of columns for displaying the group structures in the “Gamma” and “Neutron” tabs.

- **“Select Activation or Fuel Model”**

This basically sets the input units for any irradiation cases you define. In “Activation” mode, you define an irradiation by the neutron flux through the sample. “Fuel Irradiation” mode is more suited for reactor applications--you specify the neutron source strength in terms of the burnup of the uranium present.

Note that you cannot use the “Activation” mode unless ORIGEN has access to a valid activation library. Most of the data sets that ORIGEN interpolates from are based on reactor measurements and burnup. Creating such an activation library using the TRITON module is next to impossible, and by default ORIGEN-S does not have any defined.

- **“Do not warn before adding time steps to irradiation cases”**

When defining the time steps for an irradiation, you have the option to “Fill” steps up to a certain time. ARP will generate the intermediate time steps for you, but by default will ask if it's OK to create them.

- **“Always warn when enrichment is out of range for selected library”**

The data libraries used by ORIGEN are based on reactor measurements, for which Uranium enrichment is a key parameter. Most libraries have upper limits on the percentage of fissile material that can be present in the system.

Default Settings

Setup Values

Maximum number of energy groups

239

Number of columns for energy groups

10

Editor Setup

Select Activation Model or Fuel Model

☒ Fuel Irradiation Mode

☐ Activation Mode

\*\*\* WARNING \*\*\*

Setup values can ONLY be changed at startup.

Reset Defaults

☐ DO NOT WARN before adding time steps to IRRADIATION cases.

☐ ALWAYS WARN when enrichment is out of range for selected library.

?

Help

😊

OK

😊

CANCEL

## 2. COMPS

This is where you enter the concentrations of nuclides in the sample material you would like to irradiate or decay. There are two options that apply to all nuclides, and 4 that you must enter for every material component.

- **“Fuel Type”**

Selects the reactor library to use for irradiation cases. As mentioned earlier, ORIGEN-S only has geometry data for a select number of nuclear reactors. This option tells the program how to deal with neutron transport.

- **“Units”**

Fairly self-explanatory--describes the units in which composition data is entered (i.e. grams, gram-atoms, etc.)

- **“Element”**

Specify the atomic number or elemental abbreviation for the nuclide here.

- **“Isotope”**

This drop-down list lets you select from all the known isotopes of a given element. You can also select “natural” to use all the stable isotopes of an element in their natural abundances.

- **“Library”**

A nucleus will behave differently based on how it forms. Fission fragments may be excited forms of the light nuclei they share names with, for example. There are four choices in total, but ARP will only offer you those for which data is available.  $^{235}\text{U}$  is always considered an Actinide, whereas  $^{89}\text{Y}$  can be either a “Light Nucleus” or a fission product.

- **“Concentration”**

This is where you specify the amount of a nuclide that is present. Geometrical effects like density are not accounted for.

This tab also has two special buttons.

- **“Enrich”**

Provides a quick way to produce fuel of a given  $^{235}\text{U}$  enrichment. Simply specify the total amount of uranium and the  $^{235}\text{U}$  percentage, and ORIGEN-ARP will enter the appropriate amounts of the natural nuclides of uranium.

- **“Fuel Dist.”**

Allows the user to manually edit uranium isotopic abundances. Note that the total abundance must add to 100%.

OrigenArp - [Composition Data   Untitled]

File   Edit   View   Window   Help   Express

Options

new   open   save   print   help   run   output   plot   tables   editor   express

Comps

Ok   Apply   Reset   Help   Previous   Next   Enrich   Fuel Dist   Del Row   Cancel

Neutron

Enter composition data   Restart from existing data file   Units   Grams   Compositions   Irradiation Mode   Page 1

Gamma

Fuel Type   ce14x14

Cases

Moderator Density   0.733200   g/cc

Summary

Uranium   0   g

Plot Setup

Enrichment (wt%U235)   0

	Element	Isotope	Library	Concentration
1	U	235	Actinide	
2	Y	89		
3				

Ready   NUM

### 3. NEUTRON

Note that there is no way to input the energy spectra of any irradiating neutrons in ORIGEN. The reactor libraries are based on their characteristic neutron flux profiles. The neutron energy groups let you specify the coarseness of the energy binning, which affects the cross-sections used for activation reactions. For example, consider a two-group neutron structure defined:

**Group 1: 0 eV to 0.025 eV**

**Group 2: 0.025 to 100 keV**

All neutrons are then grouped into these bins, and an average cross-section is computed for each.

You can choose from 8 pre-defined neutron energy groupings, or you can define your own.

To make a custom structure, choose “Other” from the “Group Structure” drop-down list. Then specify the desired number of bins. A set of blank boxes will appear. Enter the upper energy bin boundary in eV for each bin. The last bin will always start at 0 eV.

Note that this is one of the more tedious aspects of the data entry. I will go over how to enter complex group structures directly into an ORIGEN-S input in a later section.

OrigenArp - [ Neutron Energy Spectra Untitled]

File Edit View Window Help Express

Options new open save print help run output plot tables editor express

Comps Ok Apply Reset Cancel

Neutron Group Structure 27GrpENDF4 Number of Groups 27 Neutron Energy

Maximum Neutron Energy (eV) by Group

1	2.0000000e+007	2	6.4340000e+006	3	3.0000000e+006	4	1.8500000e+006	5	1.4000000e+006
6	9.0000000e+005	7	4.0000000e+005	8	1.0000000e+005	9	1.7000000e+004	10	3.0000000e+003
11	5.5000000e+002	12	1.0000000e+002	13	3.0000000e+001	14	1.0000000e+001	15	3.0499900e+000
16	1.7700000e+000	17	1.2999900e+000	18	1.1299900e+000	19	1.0000000e+000	20	8.0000000e-001
21	4.0000000e-001	22	3.2500000e-001	23	2.2500000e-001	24	9.9999850e-002	25	5.0000000e-002
26	3.0000000e-002	27	9.9999980e-003	28	1.0000000e-005				

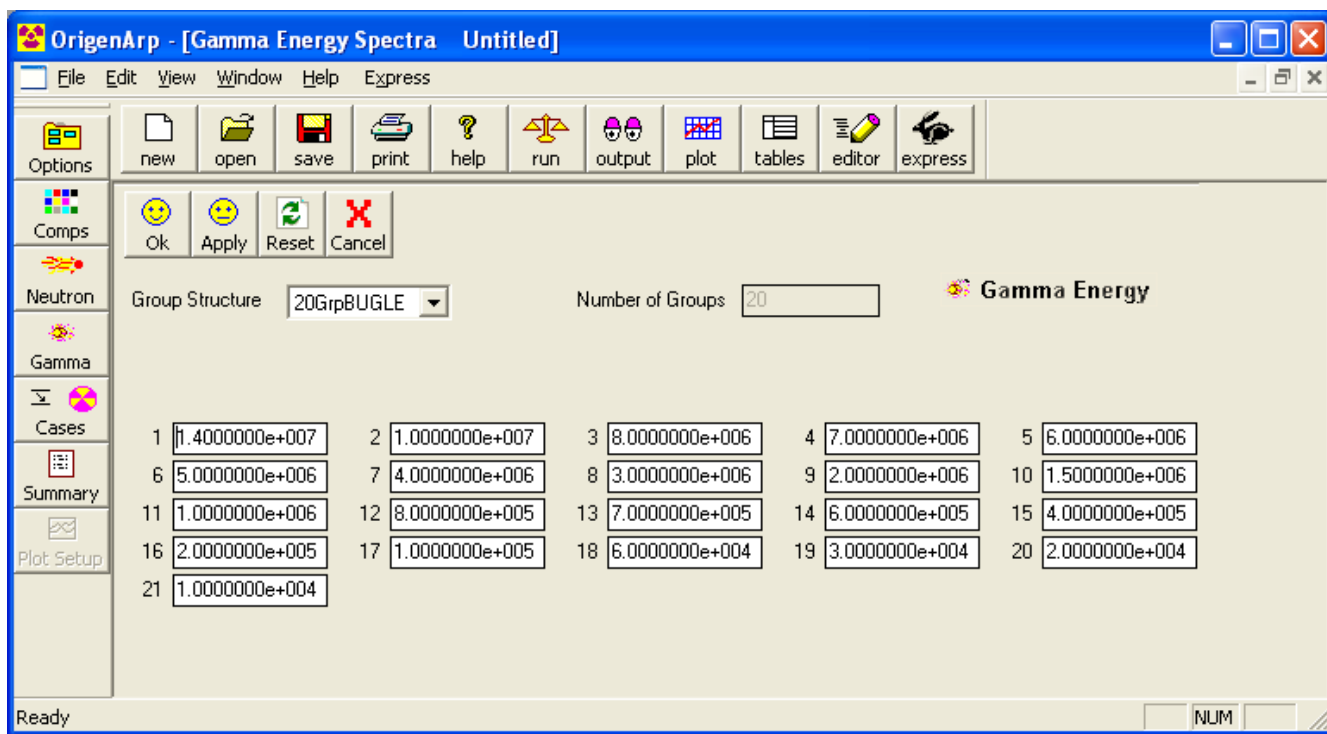
Ready NUM

## 4. GAMMA

The gamma energy groups are used for output gamma decay spectra, if you choose to save them. As with the neutron groups, there are presets for convenience (but only 5 instead of 8). You can also define your own.

To make a custom structure, choose “Other” from the “Group Structure” drop-down list. Then specify the desired number of bins. A set of blank boxes will appear. Enter the upper energy bin boundary in eV for each bin. The last bin will always start at 0 eV.

Note that this is one of the more tedious aspects of the data entry. I will go over how to enter complex group structures directly into an ORIGIN-S input in a later section.

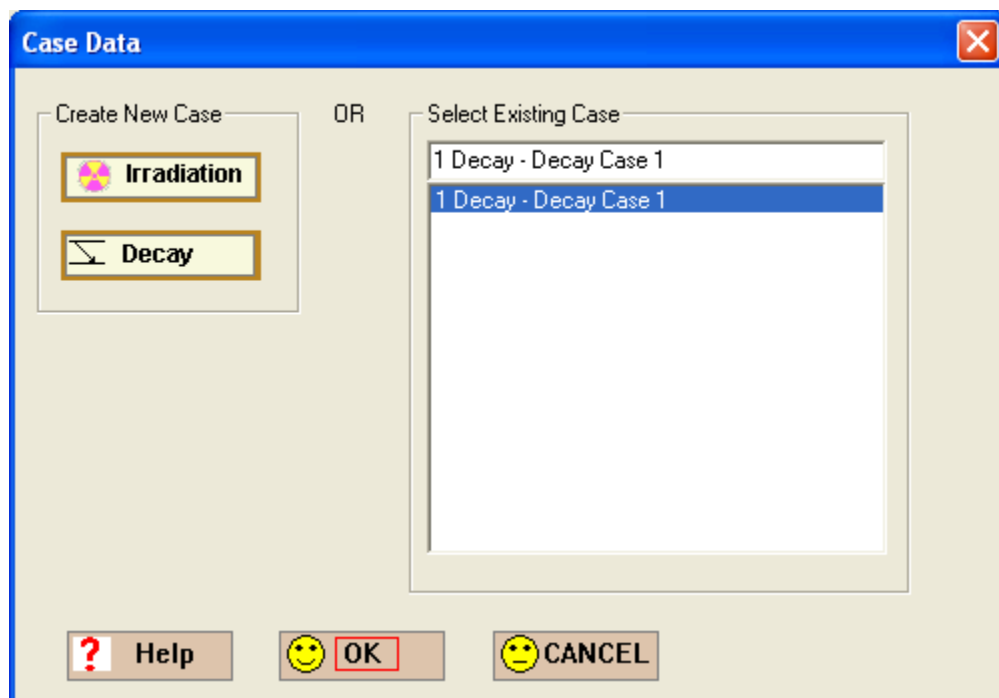


## 5. CASES

The CASES tab controls the most important aspects of an ORIGEN-S simulation. Here one defines the intensity of neutron irradiation, as well as the lengths of both cool-off and irradiation steps. Furthermore, the user also has control of the output tables from the “Options” menu that is specific to this tab.

Note: a “case” is a block of time during which either decay or irradiation occurs, but not both. They are limited to 10 smaller time steps, which are more or less arbitrarily defined.

Upon pressing the CASES tab, a menu appears where one can choose an existing decay or irradiation case to edit, or to create a new case if desired.



The above menu should be fairly self-explanatory. Note that all existing cases will appear in the list on the right side.

I will break the creation of a new case into two sub-sections: one for irradiation and the other for decay.

## IRRADIATION CASE

- **“Title”**

Every case must have a title, though it does not need to be unique.

- **“Basis”**

The basis is the amount of fissile uranium present in a sample. For “Fuel irradiation” mode, it is given in metric tons, whereas for the “Activation” mode it is given in grams. The basis serves as a normalizing factor for the intensity of irradiation. This quantity cannot be altered directly, because ORIGEN-ARP calculates it from the composition.

- **“Start all irradiation cases at time zero”**

This option applies to all irradiation cases, but is only visible for the first one. If selected, all irradiation begins concurrently with the initial composition of the material.

- **“Beginning Time”**

Each irradiation case begins where the last one left off. See the note below for a clarification of cumulative time.

- **“Time unit”**

Lengths of time steps can be entered in seconds, minutes, hours, days, or years.

The next three quantities are given for every time step in a specific case.

- **“Power (MW/Basis)” or “Flux”**

Specifies the intensity of the neutron radiation incident on the sample material during a time step. In “Fuel Irradiation” mode, this field is given in power (megawatts per metric ton uranium). For “Activation” mode, a neutron flux is given instead, with units of neutrons per cm<sup>2</sup> per second.

- **“Cumulative Time”**

This field denotes the end time for the time step. Note that cumulative times must be entered in increasing order within a case. See the note below for a clarification of cumulative time.

- **“Save Results”**

ORIGEN-S will only save output tables for which this option is selected.

A note on what ORIGEN-S means by “cumulative time”. The two types of cases occur on independent time lines, rather than sequentially. For example, suppose one specifies an irradiation case from 0 s to 100 s. If one then creates a **decay** case, it will still start at time  $t = 0$  s, rather than  $t = 100$  s. However, the next **irradiation** case will begin at  $t = 100$  s, unless the “Start all irradiation cases at time zero” option is selected.

The cumulative refers to the time that has passed since the beginning of that case, not the time since the beginning of all cases. That is, if a given case starts at  $t = 30$  days and its first time step should end 32 days after the beginning of the irradiation, then the cumulative time for that step would be 2 days.

OrigenArp - [Irradiation Case 1    Untitled]

File   Edit   View   Window   Help   Express

Options   new   open   save   print   help   run   output   plot   tables   editor   express

Comps   Ok   Apply   Reset   Help   Previous   Next   Cancel   Fill   Insert   Delete   Options   Element

Neutron

Gamma

Cases

Summary

Plot Setup

Title   Case 1

Basis   0 grams

☐ Start ALL Irradiation Cases at Time Zero

Beginning Time = 0.0      Time Units   Minutes

Flux	Cumulative Time	Save Results
4.56e+007	8	<input type="checkbox"/>
4.56e+007	16	<input type="checkbox"/>
4.56e+007	24	<input type="checkbox"/>
4.56e+007	32	<input type="checkbox"/>
4.56e+007	40	<input type="checkbox"/>
4.56e+007	48	<input type="checkbox"/>
4.56e+007	56	<input type="checkbox"/>
4.56e+007	64	<input type="checkbox"/>
4.56e+007	72	<input type="checkbox"/>
4.56e+007	80	<input type="checkbox"/>

Ready      NUM

**Irradiation**  
Case # 1

## **DECAY CASE**

- **“Title”**

Every case must have a title, though it does not need to be unique.

- **“Basis”**

The basis is the amount of fissile uranium present in a sample. For “Fuel irradiation” mode, it is given in metric tons, whereas for the “Activation” mode it is given in grams. The basis serves as a normalizing factor for the intensity of irradiation. This quantity cannot be altered directly, because ORIGIN-ARP calculates it from the composition.

- **“Beginning Time”**

Each decay case begins where the last one left off. See the note below for a clarification of cumulative time.

- **“Time unit”**

Lengths of time steps can be entered in seconds, minutes, hours, days, or years.

The next three quantities are given for every time step in a specific case.

- **“Cumulative Time”**

This field denotes the end time for the time step. Note that cumulative times must be entered in increasing order within a case. See the note below for a clarification of cumulative time.

- **“Source Spectra”**

ORIGIN-S can calculate the gamma emission spectra from nuclear decay within a material. Checking this option will save the spectrum emitted during a given time step.

- **“Save Results”**

ORIGIN-S will only save output tables for which this option is selected.

The remaining options control the secondary-particle physics for the decay case as a whole.

- **“(Alpha,n)”**

This option controls how alpha particles react in the setup matrix material. Two common reactor matrix materials are available: UO<sub>2</sub> and borosilicate glass. If the “Problem Specific” option is selected, then the matrix is assumed to be made of the sample material.

- **“(Alpha,n) Cutoff”**

Some ( $\alpha$ ,n) reactions have very small cross-sections. This option allows one to ignore reactions that are below a certain fraction of the total ( $\alpha$ ,n) contribution.

- **“Alpha Groups”**

Like the gamma and neutron groups, this controls the number of energy bins for alpha particles. The group structure for an alpha particle is broken into linearly-spaced bins from its endpoint energy down to zero energy.

- **“Bremsstrahlung”**

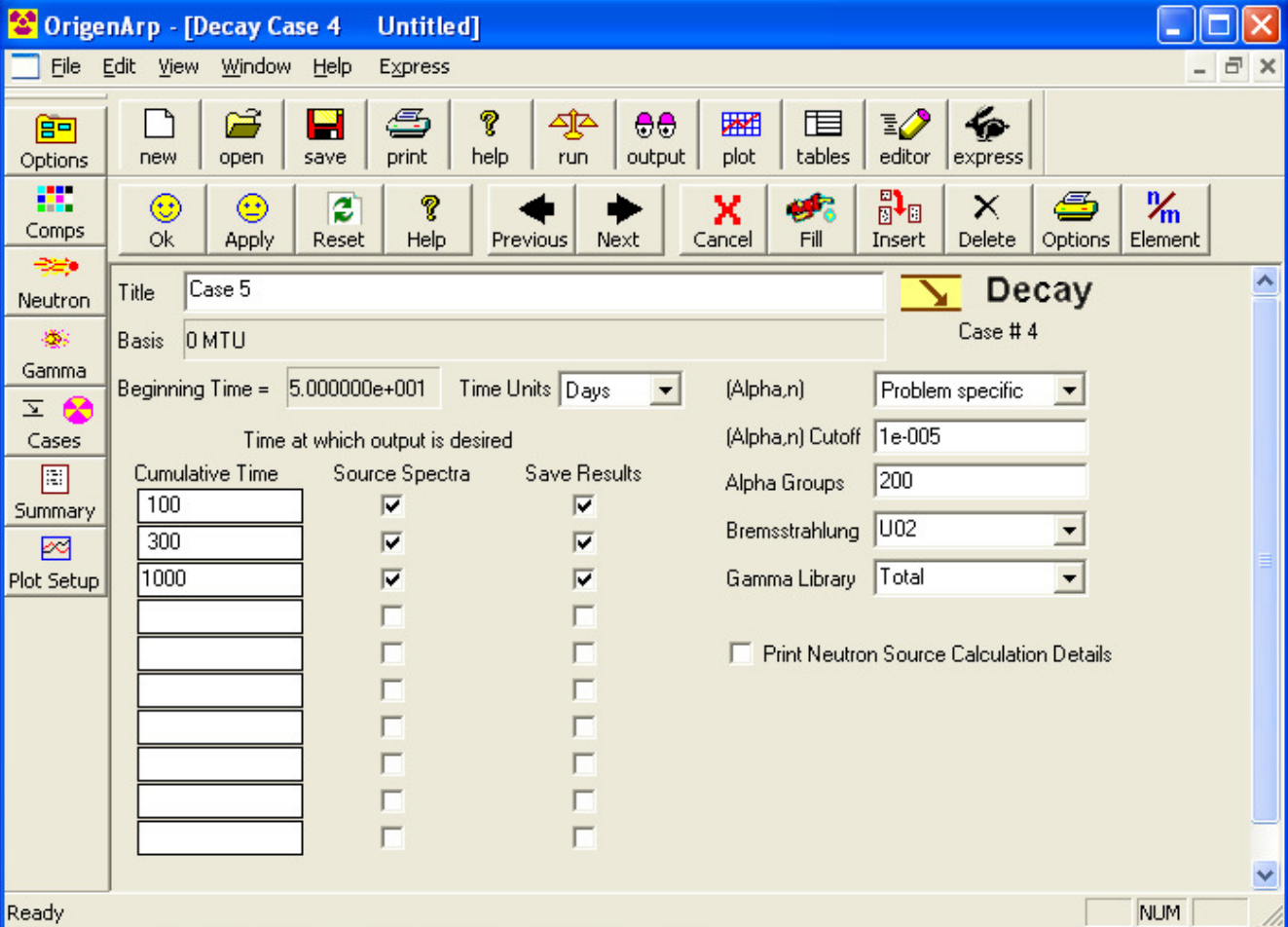
Defines the material through which beta emissions transport in the simulation. Different materials give off different bremsstrahlung radiation, based on the material density and the atomic numbers of nuclides present.

- **“Gamma Library”**

This option allows the user to ignore the gamma emissions for entire groups of nuclides. To obtain a total gamma emission spectrum, this option should be set to “Total”.

- **“Print neutron source calculation details”**

If selected, ORIGIN specifies where secondary neutrons produced in the material came from.



Note the special buttons available for the “Cases” tab.

- **“Previous” and “Next”**

For navigating between the different cases specified in the file.

- **“Fill”**

For easily entering cumulative times for many time steps. The use of this feature is different for irradiation and decay cases. See the note below for clarification.

- **“Insert”**

Creates a case in between two existing ones. ARP will not shift the cumulative times of pre-existing steps accordingly, so beware.

- **“Delete”**

Brings up a drop-down list of cases that can be deleted.

- **“Options”**

There are several further parameters than can be set in the “Options” window. Keep in mind that these apply to all cases of a given type.

- **“Table Cutoff”**

Controls the sensitivity of output results. Nuclides that are below a fraction of the total mass of the system are not written to output tables.

- **“Output Precision”**

Specifies the number of decimal places to use in the output tables.

- **“Results in”**

Gives the units of the output tables (i.e. grams, curies, etc.).

- **“Tables”**

Selects which output tables to print. One can choose Nuclides, Elements, and Summary tables. A summary table contains data for both nuclides and elements.

- **“Edit By”**

ORIGEN classifies the various nuclides into three main groups: Light Nuclei, Fission Products, and Actinides. This option specifies which groups should be saved to a table.

- **“Element”**

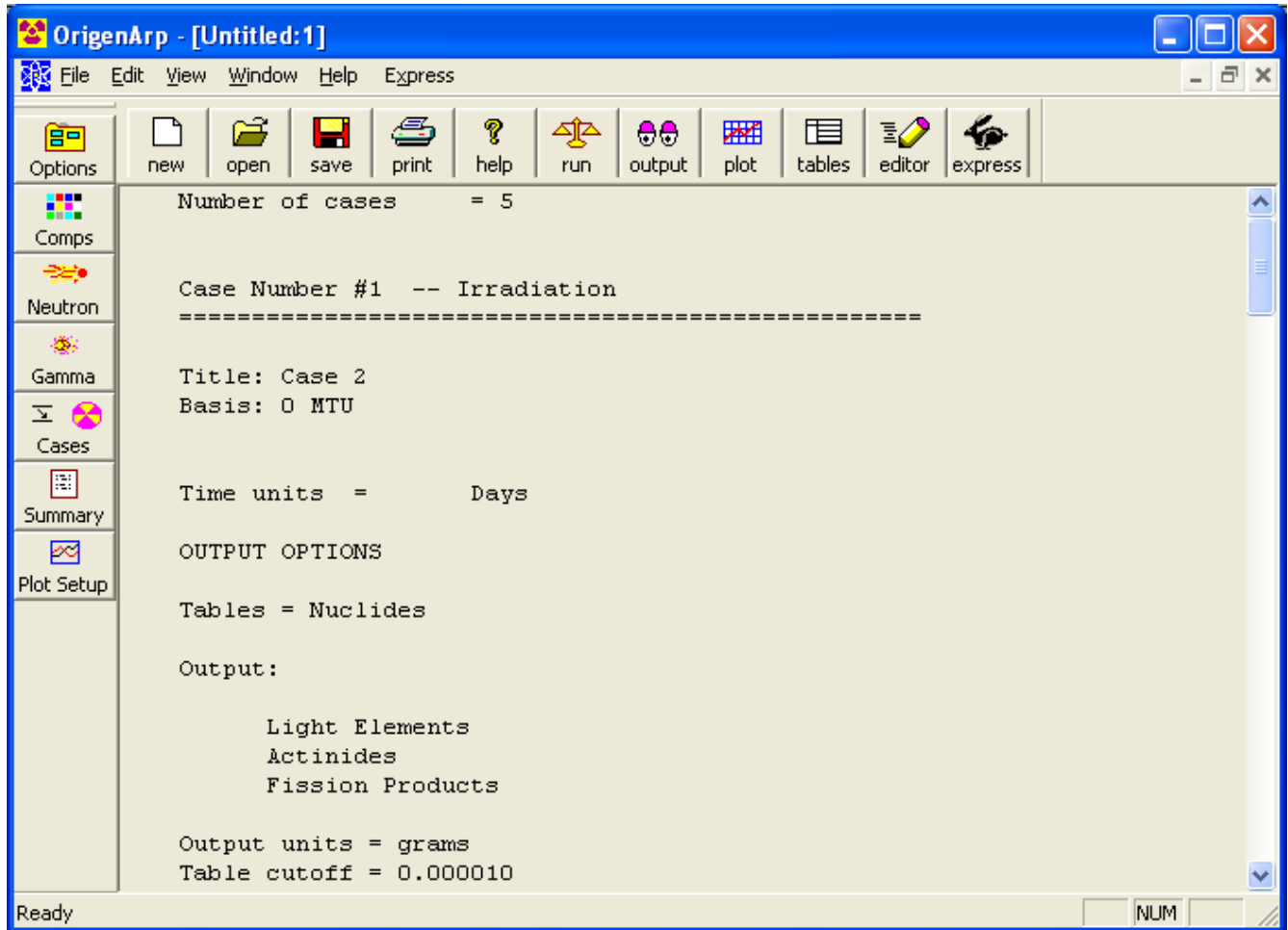
Allows the user to remove fractions of any element from the system. ORIGEN will keep the specified fraction of an element in the system, and discard the rest. Only available for decay cases.

A note on the “Fill” feature. For an irradiation case, input the desired neutron source strength (in burnup or flux) and the desired end time in the first line. Pressing “Fill” will cause ARP to create time steps (and extra cases) as necessary to obtain accurate results up to the time specified. The source strength and the “Save Results” fields will be copied to every new time step. New time steps will be spaced no more than 100 time units apart. For example, filling to 8000 days of irradiation will create 80 new time steps, split between 8 sequential irradiation cases.

For a decay case, one only need enter the desired cumulative time in the first row. ARP will fill up to this time using its so-called “rule of threes”, by which each time step is three times as long as the one preceding it, until the desired time is reached. For example, filling to 8000 days of decay would add time steps at 1 day, 3 days, 10 days, 30 days, 100 days, 300 days, 1000 days, 3000 days, and finally 8000 days. The first time step will be scaled so that the fill only takes up a single decay case. Similarly to the irradiation mode, the “Source Spectra” and “Save Results” options specified in the fill step are copied to each of the new steps.

## 6. SUMMARY

This section does not provide any data input, but rather supplies the user with details of the ORIGIN simulation, using data entered in the other main sections.



## 7. PLOT SETUP

The Plot Setup menu allows convenient output of ORIGEN data in the form of plotOPUS tables. Both time-dependent compositions and gamma emission spectra can be printed using this tool. The plots are saved after the ORIGEN-S calculations within the same output file. In addition, plotOPUS produces files containing visual representations of the data. Note that plotOPUS graphs are limited between 1 and 1000 data points. Also, ORIGEN-ARP limits the user to plotting 80 time steps. One can overcome this arbitrary hurdle by manually editing the ORIGEN-S input deck.

First, pick a plot to edit from the “Select Plot” drop-down menu. Only plots that have been initialized will appear as choices. One must click the button labeled “New” to initialize more plots.

Specific plot types come with different options. The “Plot Type” box lists the 6 supported output tables that plotOPUS can extract from ORIGEN-S.

- **“Nuclides”**

Lists the concentrations of nuclides present in the sample material as a function of time.

- **“Elements”**

Similar to the nuclide plot, except that all isotopes of a given element are grouped into one tally.

- **“Gamma Spectra”**

Provides the emission spectra for gamma rays for each time step in the selected range of decay cases. (Not available for irradiation cases.)

- **“Total Neutron Spectra”**

Like the emitted gamma spectra, this plot type is only available to decay cases.

- **“(Alpha,n) Reactions”**

Details the frequency and type of ( $\alpha$ ,n) reactions within the matrix material.

- **“Spontaneous Fission”**

Lists the counts and sources of spontaneous fission within the source material.

The “Nuclides” and “Elements” plots use the most options, and are very similar in format.

- **“Case type”**

plotOPUS saves results for irradiation and decay cases separately. This option selects between the two.

- **“Cases to Plot”**

One can choose to plot composition data for all cases of one type, or for single cases at a time.

- **“Output Units”**

The composition can be output in a variety of units, such as grams, gram-atoms, becquerels, etc.

- **“Library Type”**

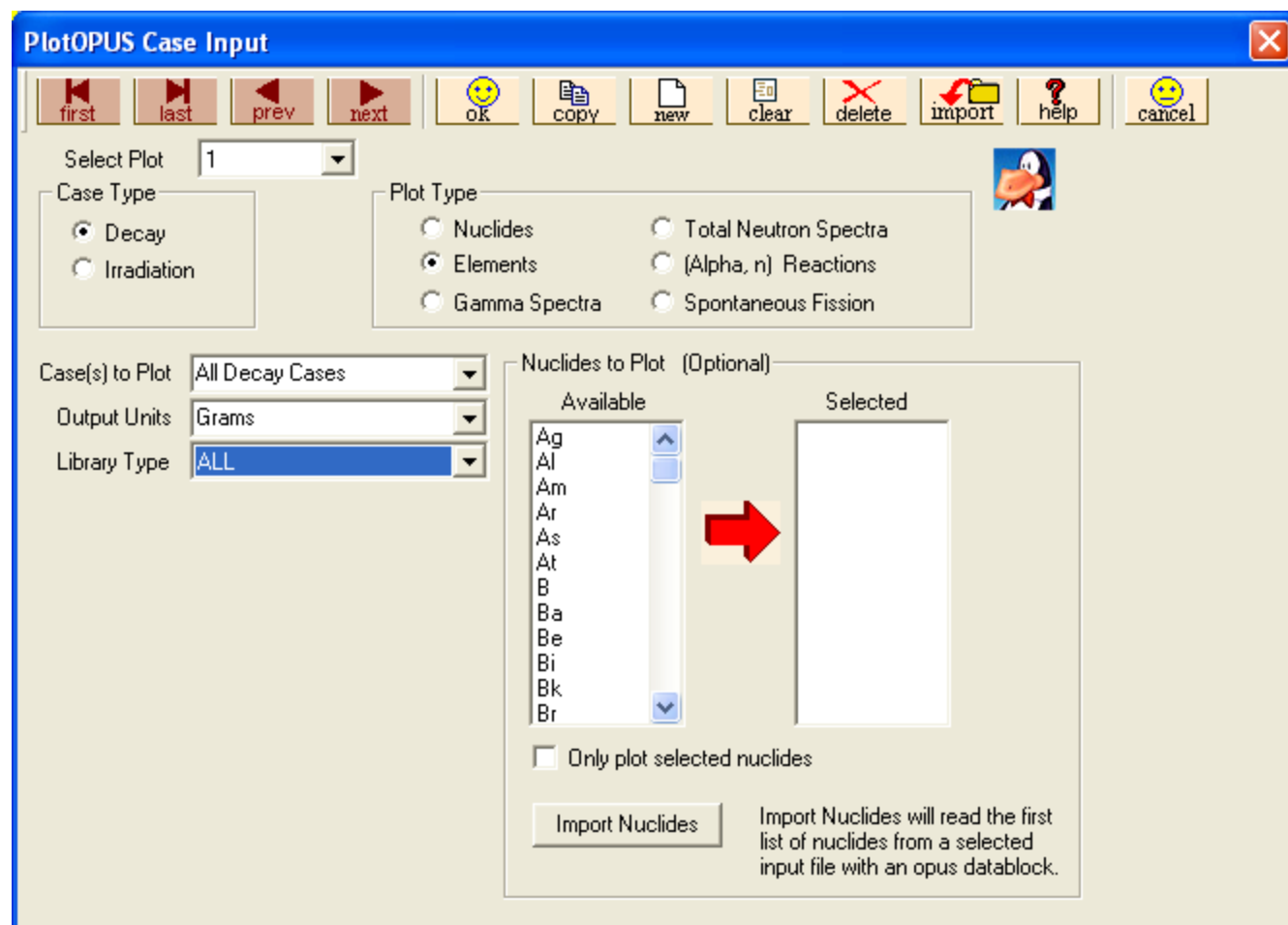
ORIGEN-S groups nuclides into 3 groups: Actinides, Light Nuclei, and Fission Products. One can choose to plot only nuclides from select groups, or simply save results for all tracked nuclides.

- **“Nuclides to Plot (Optional)”**

This is a refinement of the “Library Type” option, which allows the user to request composition data for specific elements and nuclides. If the “Only plot selected nuclides” box is left unchecked, then all available nuclides from the selected libraries are plotted.

The other four plot types have fewer parameters. For the “Total Neutron Spectra”, “(Alpha,n) Reactions”, and “Spontaneous Fission” types, only the “Cases to Plot” option is available.

The “Gamma Spectra” plot has two options: “Cases to Plot” and “Units”. Using units of photons / s / MeV gives a standard plot of countrate, normalized to the time and energy bin widths. One can also obtain plots of total energy released per time and energy bin, with the energy / s / MeV unit.



The image shows the "PlotOPUS Case Input" dialog box. It features a toolbar at the top with buttons for navigation (first, last, prev, next), actions (OK, copy, new, clear, delete, import, help, cancel), and a penguin icon. The main area contains several sections: "Select Plot" with a dropdown set to "1"; "Case Type" with radio buttons for "Decay" (selected) and "Irradiation"; "Plot Type" with radio buttons for "Nuclides", "Elements" (selected), "Gamma Spectra", "Total Neutron Spectra", "(Alpha, n) Reactions", and "Spontaneous Fission"; "Case(s) to Plot" with a dropdown set to "All Decay Cases"; "Output Units" with a dropdown set to "Grams"; and "Library Type" with a dropdown set to "ALL". A section titled "Nuclides to Plot (Optional)" contains two lists: "Available" (listing elements from Ag to Br) and "Selected" (empty), with a red arrow pointing from Available to Selected. Below these lists is a checkbox "Only plot selected nuclides" (unchecked) and an "Import Nuclides" button. A text box explains: "Import Nuclides will read the first list of nuclides from a selected input file with an opus datablock."

**PlotOPUS Case Input**

first last prev next OK copy new clear delete import help cancel

Select Plot: 1

Case Type:  
☒ Decay  
☐ Irradiation

Plot Type:  
☐ Nuclides  
☒ Elements  
☐ Gamma Spectra  
☐ Total Neutron Spectra  
☐ (Alpha, n) Reactions  
☐ Spontaneous Fission

Case(s) to Plot: All Decay Cases

Output Units: Grams

Library Type: ALL

Nuclides to Plot (Optional)

Available: Ag, Al, Am, Ar, As, At, B, Ba, Be, Bi, Bk, Br

Selected:

☐ Only plot selected nuclides

Import Nuclides

Import Nuclides will read the first list of nuclides from a selected input file with an opus datablock.

## DATA ENTRY IN ORIGEN-S

Data entry can become quite tedious in the ARP interface. For example, defining very complex compositions or energy groupings could take hours when using drop-down menus and text boxes. Even defining multiple decay or irradiation cases with mouse clicks can become irksome. Editing the ORIGEN-S input file by hand can speed up the process, but one must know all the parameters to change for a given task. For example, if one fails to specify the number of nuclides present in the initial composition, execution of ORIGEN-S will throw an error.

Also, be wary of the 80-character line limit! Exceeding this boundary may not result in an execution error, but all information beyond the 80th column is treated as a comment. I once ran into a problem where the gamma emissions were 20 orders of magnitude higher than I expected. Turns out that a line in my composition definition went beyond 80 characters, so that ORIGEN registered 1.99E-2 grams of a highly radioactive nuclide, instead of the 1.99E-21 grams I intended!

I have dedicated this last section to editing ORIGEN-S input decks manually. It is helpful to use ORIGEN-ARP to generate a skeleton, and then change a few lines. Most of the edits would also benefit from computer automation in the form of a Python script or similar. If you need an example of such a script, I have implemented each of the following in the Delayed Gamma Simulator (written in Python).

Note that ORIGEN may run out of memory when dealing with detailed compositions or energy group structures. By default, the program only requests the use of 300K of memory, and will crash if it exceeds this limit. You can fix this by adding a single line to an input file, right above the 0\$\$ vector:

**-1\$\$ [MEMORY]**

where MEMORY represents the amount of storage space requested, in bytes. I commonly set MEMORY at 20000000.

Recall that vectors in ORIGEN-S are simply sequences of parameters, with entries separated by single spaces. Special notation allows you to use the defaults for many entries in a row. For vectors longer than 80 characters, split the vector into multiple lines. All lines beyond the first, and until the end of the vector, should start with at least one blank space.

## 1. DEFINING THE INITIAL COMPOSITION

The initial composition is defined once in the file, in the first decay or irradiation case. There are three vectors that specify the composition, each of which must be the same length. The entries within these vectors line up, so that the jth ZAID corresponds to the jth mass and the jth library ID.

In addition, one must input the total number of nuclides initially present in a separate vector near the beginning of the file.

- **Vector 73\$\$**

A list of the ZAIDs for nuclides in the material, given in the ORIGEN standard. For example, one would use “922350” for the ground state of <sup>235</sup>U and “471011” for an excited state of <sup>101</sup>Ag.

- **Vector 74\*\***

Defines the amounts of each nuclide present. The units of this array are specified in the 3\$\$ array, at the 16th position. Use the following values when setting this parameter:

- 0: gram-atoms
- 1: weight in parts per million (ppm)
- 2: grams
- 3: atoms in parts per million (ppm)
- 4: curies

- **Vector 75\$\$**

Sets the library to use for a given nuclide. One advantage of ORIGEN-ARP is that it will automatically rule out invalid libraries when selecting from the drop-down list it provides for composition input. (See the note below.)

There are four library choices, corresponding to the following numerical designations:

- 1: Light Element
- 2: Actinide
- 3: Fission Product
- 4: Light Element, when using relative abundance

- **Vector 56\$\$**

This vector stores quite a few parameters, and is also somewhat ambiguous in its use. It appears several times in the file, but only the first instance contains data we need to edit manually. One of the middle entries specifies the number of nuclides present, which should match the length of the 73\$\$, 74\*\*, and 75\$\$ vectors. See below for an example.

If a library is missing data for a nuclide, ORIGEN will simply ignore that nuclide in its calculations, and give a warning in the output file. After some trial and error, I was able to extract the correct libraries for a large number of fission products from these warning messages. I wrote the results into a set of files, which the Delayed Gamma Simulator uses to create an appropriate vector 75\$\$ for the composition.

The 56\$\$ array has a couple forms, depending on where it appears in the file. The first one corresponds to the initial conditions for the simulation, and may be something like:

```
56$$ a2 10 a6 1 a10 0 a13 [NUCLIDES] a14 1 a15 3 a17 2 e
```

The parameter marked NUCLIDES is where you would input the length of your composition vectors. Farther in the input, the 56\$\$ array appears once for each time step, in the form

```
56$$ 0 0 a10 [XXX] e t
```

where XXX represents the position of the time step within a case. (So, XXX ranges from 1 to 10, since there can be 10 time steps per case.) These 56\$\$ arrays for time steps need not be edited once ORIGEN-ARP creates them.

## 2. SETTING THE PHOTON GROUP STRUCTURE

The default photon group structures used for output gamma emission spectra are generally very coarse. Should one want to investigate the behavior of a specific decay line over time, one must define a custom set of energy bins. This can be done within ORIGEN-ARP, but becomes impractical for very fine bins (say, 1keV from 0 keV to 3 MeV).

The annoying thing about editing the photon groups by hand is that the groups are defined separately for each and every decay and irradiation case. Input for these groups is contained in vector 83\*\*.

In addition to editing all the 83\*\* vectors in a file, one must also change a single setting in the 3\$\$ vector, which is located at the beginning of an input file. It looks like this:

```
3$$ 21 1 1 0 a16 2 a33 [E_BINS-1] e t
```

where “E\_BINS - 1” is the number of photon groups, minus one.

Recall that group structures are listed in monotonically decreasing order, with the energies given in eV. Each entry corresponds to the upper boundary for a group.

### 3. ADDING A DECAY CASE

A decay case is governed by a couple dozen lines of input. Luckily, the vast majority of each is static, and need not be changed from one case to the next. The text below shows all the lines defining a decay case, with some substitutions made where parameters must be changed.

```
56$$$ a2 10 a6 1 a10 10 a14 1 a15 3 a17 2 e
57** [START_TIME] a3 1e-05 e
95$$$ 0 t
[TITLE]
0 MTU
60** [TIMES]
61** f1E-24
65$$$
'Gram-Atoms      Grams      Curies      Watts-All      Watts-Gamma
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
 3z   1   0   0   3z   3z   3z   6z
81$$$ 2 0 26 1 e
82$$$ 2 2 2 2 2 2 2 2 2 2 e
83** [ENERGY_BINS] e
t
56$$$ 0 0 a10 1 e t
56$$$ 0 0 a10 2 e t
56$$$ 0 0 a10 3 e t
56$$$ 0 0 a10 4 e t
56$$$ 0 0 a10 5 e t
56$$$ 0 0 a10 6 e t
56$$$ 0 0 a10 7 e t
56$$$ 0 0 a10 8 e t
56$$$ 0 0 a10 9 e t
56$$$ 0 0 a10 10 e t
54$$$ a8 1 a11 0 e
```

In total, there are four lines that should be changed from case to case.

- In vector 57\*\*, the START\_TIME parameter gives the cumulative time for which the previous decay case ended.
- The TITLE line, not a vector itself, is simply a label for the decay case.
- The 60\*\* vector is the really critical piece, since it defines the cumulative times for each of the time steps in the case. If there are X time steps, there should be X entries here. Also note that all cases except the last must have 10 time steps.
- Finally, in vector 83\*\*, one should replace ENERGY\_BINS with the gamma group structure, in descending order and listed in eV.

## 4. PLOTTING FOR MORE THAN 80 TIME STEPS

As mentioned earlier, when using the Plot Setup provided in ORIGEN-ARP, the editor will give an error if you try to plot more than 80 time steps. This is an arbitrary limitation which is fairly easy to address. The following lines control a 200 time-step plotOPUS gamma spectrum plot:

```
=opus
LIBUNIT=21
TYPARAMS=GSPECTRUM
UNITS=GRAMS
TIME=SEC
NPOSITION=1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48
49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96
97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115
116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133
134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151
152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169
170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187
188 189 190 191 192 193 194 195 196 197 198 199 200 end
end
```

Each entry in NPOSITION corresponds to a different time step to plot data for. Since this is a long vector (more than 80 characters), it is broken into several lines. Each subsequent line starts with a blank space.

# AN ORIGEN-S SKELETON

To wrap up, I will include a sample skeleton file with all the important parameters undefined (in **bold**). This skeleton defines a simple decay with no irradiation cases.

```
'This SCALE input file was generated by
'OrigenArp Version  5.1.01 March 22, 2007
#origens
-1$$ [MEMORY]
0$$ a11 71 e t
Decay Case
3$$ 21 1 1 0 a16 [COMPOSITION_UNITS] a33 [E_BINS-1] e t
35$$ 0 t
54$$ a8 1 a11 0 e
56$$ a2 10 a6 1 a10 0 a13 [NUCLIDES] a15 3 a17 2 e
57** 0 a3 1e-05 e
95$$ 0 t
[TITLE]
[BASIS]
60** [TIME_STEPS]
61** f0.05
65$$
'Gram-Atoms    Grams    Curies    Watts-All    Watts-Gamma
 3z   1    0    0   3z   3z   3z   6z
 3z   1    0    0   3z   3z   3z   6z
 3z   1    0    0   3z   3z   3z   6z
81$$ 2 0 26 1 e
82$$ 2 2 2 2 2 2 2 2 2 2 e
83**
[ENERGY_BINS] e
73$$ [NUCLIDE_ZAIDS]
74** [NUCLIDE_MASSES]
75$$ [NUCLIDE_LIBRARIES]
t
56$$ 0 0 a10 1 e t
56$$ 0 0 a10 2 e t
56$$ 0 0 a10 3 e t
56$$ 0 0 a10 4 e t
56$$ 0 0 a10 5 e t
56$$ 0 0 a10 6 e t
56$$ 0 0 a10 7 e t
56$$ 0 0 a10 8 e t
56$$ 0 0 a10 9 e t
56$$ 0 0 a10 10 e t
56$$ f0 t
end
=opus
LIBUNIT=21
TYPARAMS=NUCLIDES
UNITS=GRAMS
LIBTYPE=ALL
TIME=DAYS
NPOSITION=[STEPS_TO_PLOT] end
end
#shell
copy ft71f001 "C:\Documents and Settings\User\Desktop\test.f71"
del ft71f001
end
```